Subject: extension of substructure definition
Posted by nbehrnd on Thu, 24 Aug 2023 09:33:37 GMT
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Dear Thomas,

I would like to suggest to extend the sketcher's functionality to define motifs.

While editing a list of motifs eventually to be used as a reference set for the evolutionary library generation, I noticed the short cut `Ctrl + double left mouse click` to define one site to be e.g., either a nitrogen, or an oxygen atom currently works only if the structure in the DW's cell already carries a similar flexibility (cf. attached silent `record_1.mp4`). Instead, the whole molecule is marked. The information necessary to DW to spot potential atomic variation can be introduced by import of a .sdf with a square bracket in the corresponding line (as in the example of `compound_50.sdf`).

If not already implemented by an other command and unidentified by me, could future releases of DW provide the substructure function/atom query feature widget equally for cells about structures which still are empty (cf. second part of `record_1.mp4, and `record_2.mp4`)?

Best regards,

Norwid

File Attachments

1) compound_50.sdf, downloaded 413 times
2) nasty_functions.dwar, downloaded 423 times
3) record_1.mp4, downloaded 373 times
4) record_2.mp4, downloaded 387 times